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Supporting Information

A. [Co(3-Cl-acacen)(NH₃)₂]BPh₄

1. Table A1.
2. Atomic Coordinates
3. Bond distances and angles
4. Anisotropic displacement parameters
5. Hydrogen coordinates

B. [Co(acacen)(4-MeIm)₂]Br•1.5H₂O

1. Structure solution information and Table B1.
2. Atomic coordinates
3. Bond distances and angles
4. Anisotropic displacement parameters
5. Hydrogen coordinates

Table A1. Crystal data and structure refinement for [Co(3-Cl-acacen) (NH₃)₂]BPh₄

Identification code	AGB1
Empirical formula	C ₃₆ H ₄₂ BCl ₂ CoN ₄ O ₂
Formula weight	703.38
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 2(1)/m (#11)
Unit cell dimensions	a = 9.720(2) Å alpha = 90° b = 18.142(4) Å beta = 100.11(3)° c = 10.046(2) Å gamma = 90°
Volume, Z	1744.0(6) Å ³ , 2
Density (calculated)	1.339 g/cm ³
Absorption coefficient	6.83 cm ⁻¹
F(000)	736
Crystal size	0.18 x 0.30 x 0.38 mm
θ range for data collection	2.06 to 19.98°
Limiting indices	-9 ≤ h ≤ 9, -17 ≤ k ≤ 17, 0 ≤ l ≤ 9
Reflections collected	3851
Independent reflections	1694 (R _{int} = 0.0330)
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1692 / 0 / 206
Goodness-of-fit on F ²	2.642
Final R indices [I > 2σ(I)]	R1 = 0.0617, wR2 = 0.1104
R indices (all data)	R1 = 0.0831, wR2 = 0.1139
Largest diff. peak and hole	0.860 and -0.473 eÅ ⁻³

Table A2. Atomic coordinates [$\times 10^4$] and equivalent isotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for [Co(3-Cl-acacen)(NH₃)₂]BPh₄. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co	1660 (1)	2500	6173 (1)	49 (1)
Cl(1)	1657 (4)	-216 (1)	5991 (3)	193 (2)
N(1)	881	1778	7179	76 (2)
N(1B)	881	3222	7179	76 (2)
O(1)	2459 (4)	1804 (3)	5148 (4)	57 (1)
N(2)	3428 (6)	2500	7442 (6)	59 (2)
N(3)	-34 (6)	2500	4790 (6)	67 (2)
C(3)	919 (9)	1086 (5)	7027 (8)	91 (3)
C(2)	1606 (11)	741 (4)	6088 (12)	97 (3)
C(1)	2371 (8)	1098 (5)	5217 (8)	73 (2)
C(4)	449	2025	8433	91 (3)
C(4B)	-36	2789	7974	91 (3)
C(5)	155 (10)	586 (6)	7897 (9)	190 (6)
C(6)	3177 (8)	703 (4)	4274 (8)	112 (3)
C(20)	-4130 (7)	1793 (3)	351 (6)	49 (2)
C(21)	-5402 (7)	1494 (4)	580 (7)	64 (2)
C(22)	-6096 (8)	936 (5)	-200 (9)	86 (3)
C(23)	-5574 (11)	652 (5)	-1263 (10)	95 (3)
C(24)	-4349 (10)	919 (5)	-1554 (7)	80 (2)
C(25)	-3636 (7)	1490 (4)	-765 (7)	62 (2)
C(40)	-1681 (9)	2500	1299 (8)	51 (3)
C(41)	-891 (7)	1853 (4)	1451 (5)	59 (2)
C(42)	563 (8)	1850 (5)	1736 (6)	75 (2)
C(43)	1299 (12)	2500	1877 (10)	87 (4)
C(30)	-3573 (8)	2500	2777 (9)	52 (3)
C(31)	-3557 (7)	1856 (4)	3527 (7)	68 (2)
C(32)	-3522 (7)	1849 (5)	4923 (7)	84 (3)
C(33)	-3529 (10)	2500	5611 (11)	83 (4)
B	-3390 (11)	2500	1196 (10)	45 (3)

Table A3. Bond lengths [Å] and angles [°] for [Co(3-Cl-acacen)(NH₃)₂]BPh₄.

Co-O(1)#1	1.881(4)	Co-O(1)	1.881(4)
Co-N(1)#1	1.8918(9)	Co-N(1)	1.8918(9)
Co-N(1B)	1.8918(9)	Co-N(1B)#1	1.8918(9)
Co-N(2)	1.951(6)	Co-N(3)	1.960(6)
Cl(1)-C(2)	1.740(8)	N(1)-N(1B)#1	0.00
N(1)-C(3)	1.267(10)	N(1)-C(4)	1.4655(3)
N(1)-C(4B)#1	1.5152(3)	N(1B)-N(1)#1	0.00
N(1B)-C(3)#1	1.267(10)	N(1B)-C(4)#1	1.4655(3)
N(1B)-C(4B)	1.5152(3)	O(1)-C(1)	1.286(8)
N(2)-H(2A)	0.89	N(2)-H(2B)	0.89
N(2)-H(2C)	0.89	N(3)-H(3A)	0.89
N(3)-H(3B)	0.89	N(3)-H(3C)	0.89
C(3)-N(1B)#1	1.267(10)	C(3)-C(2)	1.396(11)
C(3)-C(5)	1.538(10)	C(2)-C(1)	1.403(11)
C(1)-C(6)	1.512(9)	C(4)-C(4B)#1	0.6868(2)
C(4)-N(1B)#1	1.4655(3)	C(4)-C(4B)	1.5102(3)
C(4)-C(4)#1	1.7239(3)	C(4B)-C(4)#1	0.6868(2)
C(4B)-C(4B)#1	1.0493(2)	C(4B)-N(1)#1	1.5152(3)
C(5)-H(5A)	0.96	C(5)-H(5B)	0.96
C(5)-H(5C)	0.96	C(6)-H(6A)	0.96
C(6)-H(6B)	0.96	C(6)-H(6C)	0.96
C(20)-C(21)	1.405(8)	C(20)-C(25)	1.407(8)
C(20)-B	1.634(8)	C(21)-C(22)	1.381(9)
C(21)-H(21)	0.93	C(22)-C(23)	1.362(10)
C(22)-H(22)	0.93	C(23)-C(24)	1.364(10)
C(23)-H(23)	0.93	C(24)-C(25)	1.409(9)
C(24)-H(24)	0.93	C(25)-H(25)	0.93
C(40)-C(41)#1	1.395(7)	C(40)-C(41)	1.395(7)
C(40)-B	1.646(13)	C(41)-C(42)	1.392(9)
C(41)-H(41)	0.93	C(42)-C(43)	1.373(8)
C(42)-H(43)	0.93	C(43)-C(42)#1	1.373(8)
C(43)-H(43)	0.93	C(30)-C(31)#1	1.389(7)
C(30)-C(31)	1.389(7)	C(30)-B	1.629(13)
C(31)-C(32)	1.397(9)	C(31)-H(31)	0.93
C(32)-C(33)	1.368(8)	C(32)-H(32)	0.93
C(33)-C(32)#1	1.368(8)	C(33)-H(33)	0.93
B-C(20)#1	1.634(8)		
O(1)#1-Co-O(1)	84.3(3)	O(1)#1-Co-N(1)#1	94.06(14)
O(1)-Co-N(1)#1	178.4(2)	O(1)#1-Co-N(1)	178.4(2)
O(1)-Co-N(1)	94.06(14)	N(1)#1-Co-N(1)	87.58(5)
O(1)#1-Co-N(1B)	94.06(14)	O(1)-Co-N(1B)	178.4(2)
N(1)#1-Co-N(1B)	0.0	N(1)-Co-N(1B)	87.58(5)
O(1)#1-Co-N(1B)#1	178.4(2)	O(1)-Co-N(1B)#1	94.06(14)
N(1)#1-Co-N(1B)#1	87.58(5)	N(1)-Co-N(1B)#1	0.0
N(1B)-Co-N(1B)#1	87.58(5)	O(1)#1-Co-N(2)	87.5(2)
O(1)-Co-N(2)	87.5(2)	N(1)#1-Co-N(2)	92.3(2)
N(1)-Co-N(2)	92.3(2)	N(1B)-Co-N(2)	92.3(2)
N(1B)#1-Co-N(2)	92.3(2)	O(1)#1-Co-N(3)	89.3(2)
O(1)-Co-N(3)	89.3(2)	N(1)#1-Co-N(3)	90.74(14)
N(1)-Co-N(3)	90.74(14)	N(1B)-Co-N(3)	90.74(14)
N(1B)#1-Co-N(3)	90.74(14)	N(2)-Co-N(3)	175.8(3)
N(1B)#1-N(1)-C(3)	7(10)	N(1B)#1-N(1)-C(4)	107.767(5)
C(3)-N(1)-C(4)	115.2(4)	N(1B)#1-N(1)-C(4B)#1	121.179(8)
C(3)-N(1)-C(4B)#1	127.6(4)	C(4)-N(1)-C(4B)#1	26.576(11)
N(1B)#1-N(1)-Co	134(10)	C(3)-N(1)-Co	126.8(4)
C(4)-N(1)-Co	116.75(3)	C(4B)#1-N(1)-Co	104.54(3)
N(1)#1-N(1B)-C(3)#1	173(10)	N(1)#1-N(1B)-C(4)#1	72.232(5)
C(3)#1-N(1B)-C(4)#1	115.2(4)	N(1)#1-N(1B)-C(4B)	58.820(8)

C(3)#1-N(1B)-C(4B)	127.6(4)	C(4)#1-N(1B)-C(4B)	26.576(11)
N(1)#1-N(1B)-Co	46(8)	C(3)#1-N(1B)-Co	126.8(4)
C(4)#1-N(1B)-Co	116.75(3)	C(4B)-N(1B)-Co	104.53(3)
C(1)-O(1)-Co	127.0(5)	Co-N(2)-H(2A)	109.47(2)
Co-N(2)-H(2B)	109.5(2)	H(2A)-N(2)-H(2B)	109.5
Co-N(2)-H(2C)	109.5(2)	H(2A)-N(2)-H(2C)	109.5
H(2B)-N(2)-H(2C)	109.5	Co-N(3)-H(3A)	109.5(2)
Co-N(3)-H(3B)	109.5(2)	H(3A)-N(3)-H(3B)	109.5
Co-N(3)-H(3C)	109.471(13)	H(3A)-N(3)-H(3C)	109.5
H(3B)-N(3)-H(3C)	109.5	N(1B)#1-C(3)-N(1)	0.0
N(1B)#1-C(3)-C(2)	123.7(7)	N(1)-C(3)-C(2)	123.7(7)
N(1B)#1-C(3)-C(5)	119.2(9)	N(1)-C(3)-C(5)	119.2(9)
C(2)-C(3)-C(5)	117.1(10)	C(3)-C(2)-C(1)	125.6(8)
C(3)-C(2)-C1(1)	120.5(9)	C(1)-C(2)-C1(1)	113.8(9)
O(1)-C(1)-C(2)	122.8(8)	O(1)-C(1)-C(6)	113.1(8)
C(2)-C(1)-C(6)	124.1(8)	C(4B)#1-C(4)-N(1)	80.75(2)
C(4B)#1-C(4)-N(1B)#1	80.76(2)	N(1)-C(4)-N(1B)#1	0.0
C(4B)#1-C(4)-C(4B)	37.250(2)	N(1)-C(4)-C(4B)	97.988(10)
N(1B)#1-C(4)-C(4B)	97.988(10)	C(4B)#1-C(4)-C(4)#1	60.588(10)
N(1)-C(4)-C(4)#1	107.767(5)	N(1B)#1-C(4)-C(4)#1	107.768(5)
C(4B)-C(4)-C(4)#1	23.339(8)	C(4)#1-C(4B)-C(4B)#1	119.412(10)
C(4)#1-C(4B)-C(4)	96.07(2)	C(4B)#1-C(4B)-C(4)	23.339(8)
C(4)#1-C(4B)-N(1)#1	72.669(13)	C(4B)#1-C(4B)-N(1)#1	121.179(8)
C(4)-C(4B)-N(1)#1	117.098(10)	C(4)#1-C(4B)-N(1B)	72.669(13)
C(4B)#1-C(4B)-N(1B)	121.180(8)	C(4)-C(4B)-N(1B)	117.098(10)
N(1)#1-C(4B)-N(1B)	0.0	C(3)-C(5)-H(5A)	109.5(4)
C(3)-C(5)-H(5B)	109.5(6)	H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5(6)	H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5	C(1)-C(6)-H(6A)	109.5(4)
C(1)-C(6)-H(6B)	109.5(4)	H(6A)-C(6)-H(6B)	109.5
C(1)-C(6)-H(6C)	109.5(5)	H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5	C(21)-C(20)-C(25)	114.4(6)
C(21)-C(20)-B	122.5(7)	C(25)-C(20)-B	122.6(7)
C(22)-C(21)-C(20)	123.1(7)	C(22)-C(21)-H(21)	118.5(5)
C(20)-C(21)-H(21)	118.5(4)	C(23)-C(22)-C(21)	120.7(8)
C(23)-C(22)-H(22)	119.7(6)	C(21)-C(22)-H(22)	119.7(5)
C(22)-C(23)-C(24)	119.5(9)	C(22)-C(23)-H(23)	120.2(6)
C(24)-C(23)-H(23)	120.2(6)	C(23)-C(24)-C(25)	120.2(8)
C(23)-C(24)-H(24)	119.9(6)	C(25)-C(24)-H(24)	119.9(5)
C(20)-C(25)-C(24)	122.1(7)	C(20)-C(25)-H(25)	119.0(4)
C(24)-C(25)-H(25)	119.0(5)	C(41)#1-C(40)-C(41)	114.4(9)
C(41)#1-C(40)-B	122.5(4)	C(41)-C(40)-B	122.5(4)
C(42)-C(41)-C(40)	123.1(7)	C(42)-C(41)-H(41)	118.5(5)
C(40)-C(41)-H(41)	118.5(4)	C(43)-C(42)-C(41)	120.6(9)
C(43)-C(42)-H(43)	119.7(6)	C(41)-C(42)-H(43)	119.7(5)
C(42)-C(43)-C(42)#1	118.3(11)	C(42)-C(43)-H(43)	120.8(6)
C(42)#1-C(43)-H(43)	120.8(6)	C(31)#1-C(30)-C(31)	114.5(8)
C(31)#1-C(30)-B	122.4(4)	C(31)-C(30)-B	122.4(4)
C(30)-C(31)-C(32)	123.2(7)	C(30)-C(31)-H(31)	118.4(4)
C(32)-C(31)-H(31)	118.4(5)	C(33)-C(32)-C(31)	119.9(9)
C(33)-C(32)-H(32)	120.1(5)	C(31)-C(32)-H(32)	120.1(5)
C(32)-C(33)-C(32)#1	119.2(11)	C(32)-C(33)-H(33)	120.4(5)
C(32)#1-C(33)-H(33)	120.4(5)	C(30)-B-C(20)	113.1(5)
C(30)-B-C(20)#1	113.1(5)	C(20)-B-C(20)#1	103.5(7)
C(30)-B-C(40)	102.7(7)	C(20)-B-C(40)	112.4(5)
C(20)#1-B-C(40)	112.4(5)		

Symmetry transformations used to generate equivalent atoms:

#1 x, -y+1/2, z

Table A4. Anisotropic displacement parameters [$\text{\AA}^2 \times 10^3$] for [Co(3-Cl-acacen)(NH₃)₂]BPh₄. The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [(ha^*)^2 U_{11} + \dots + 2hka^*b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Co	39(1)	72(1)	35(1)	0	1(1)	0
Cl(1)	197(3)	74(2)	256(4)	47(2)	-107(3)	-43(2)
O(1)	54(3)	60(3)	56(3)	-9(2)	7(2)	2(3)
N(2)	43(5)	69(6)	60(5)	0	-7(4)	0
N(3)	47(5)	114(7)	39(4)	0	7(4)	0
C(3)	71(6)	124(9)	64(6)	31(6)	-27(5)	-33(6)
C(2)	95(7)	51(6)	117(8)	29(6)	-57(6)	-33(6)
C(1)	63(6)	48(6)	89(6)	-11(6)	-40(5)	4(5)
C(5)	165(10)	253(13)	138(8)	103(9)	-13(8)	-141(10)
C(6)	107(7)	76(6)	134(8)	-51(6)	-29(6)	33(6)
C(20)	48(5)	55(5)	38(4)	5(4)	-4(4)	11(4)
C(21)	50(5)	75(6)	62(5)	12(4)	-5(4)	-10(4)
C(22)	70(6)	86(7)	87(7)	17(5)	-26(6)	-21(5)
C(23)	99(8)	74(6)	91(8)	4(6)	-44(6)	-4(6)
C(24)	102(7)	76(7)	52(5)	-11(5)	-15(5)	23(5)
C(25)	68(5)	65(5)	50(4)	1(4)	-1(4)	5(4)
C(40)	48(7)	79(8)	24(5)	0	4(5)	0
C(41)	49(5)	89(6)	38(4)	2(4)	4(4)	10(4)
C(42)	60(7)	126(9)	40(4)	7(5)	7(4)	30(5)
C(43)	47(8)	171(15)	46(7)	0	13(6)	0
C(30)	29(5)	77(8)	50(7)	0	4(5)	0
C(31)	67(5)	88(6)	47(5)	3(4)	5(4)	-5(4)
C(32)	70(6)	133(9)	48(6)	18(5)	5(4)	-18(6)
C(33)	47(7)	167(14)	38(7)	0	13(6)	0
B	37(6)	62(7)	35(6)	0	4(5)	0

Table A5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{Co}(\text{3-Cl-acacen})(\text{NH}_3)_2]\text{BPh}_4$.

	x	y	z	U(eq)
H(2A)	3665(30)	2039(2)	7681(44)	89
H(2B)	3335(18)	2759(26)	8173(25)	89
H(2C)	4090(14)	2702(28)	7050(20)	89
H(3A)	-702(21)	2246(28)	5089(25)	100
H(3B)	149(18)	2292(30)	4038(21)	100
H(3C)	-319(35)	2962(2)	4616(44)	100
H(5A)	659(10)	580(6)	8809(9)	285
H(5B)	100(10)	95(6)	7536(9)	285
H(5C)	-771(10)	772(6)	7888(9)	285
H(6A)	2655(8)	280(4)	3894(8)	167
H(6B)	4064(8)	546(4)	4768(8)	167
H(6C)	3321(8)	1030(4)	3561(8)	167
H(21)	-5794(7)	1680(4)	1291(7)	97
H(22)	-6929(8)	753(5)	3(9)	129
H(23)	-6049(11)	278(5)	-1787(10)	143
H(24)	-3983(10)	725(5)	-2274(7)	120
H(25)	-2812(7)	1672(4)	-990(7)	94
H(41)	-1358(7)	1404(4)	1357(5)	89
H(43)	1041(8)	1404(5)	1832(6)	113
H(43)	2270(12)	2500	2063(10)	131
H(31)	-3570(7)	1407(4)	3078(7)	102
H(32)	-3495(7)	1404(5)	5384(7)	127
H(33)	-3537(10)	2500	6535(11)	125

Crystallographic Data and Structure Analysis for [Co(acacen)(4-MeIm)₂]Br•1.5H₂O

A dark brown single crystal of the complex was mounted on the Phillips PW 1100/20 Four Circle Diffractometer and accurate cell parameters were obtained from 25 centered reflections using graphite monochromated Mo K α radiation. Intensities were collected using the $\omega/2\theta$ method. Three standard reflections were monitored every 120 min. and variations in intensities no higher than 5% were observed. Intensities were corrected for Lorentz, polarization and background effects but not for absorption, and reduced to observed structure factors.

The Co and Br atoms were located by direct methods using the SHELXS-86 program and the remaining C,N and O atoms by successive Fourier difference maps using SHELXL-93. All non hydrogen atoms were refined anisotropically. Hydrogens were placed at calculated positions and refined isotropically. Other details of structure refinement are shown in Table B1.

The structure accommodates two Co complex cations, two Br anions and three solvate molecules of water in the asymmetric unit. In the structure, there are discrete hydrogen bonded clusters of Br₄•(H₂O)₆ located on inversion centers at the corners of the unit cell. The cluster is built up of three parallelograms, each having two Br ions and two water molecules occupying its opposite corners. each Br ion uses its four electron pairs to make hydrogen bonds to four water molecules, whereas each water molecule makes only two hydrogen bonds to two Br ions as a donor. The Br...H--OW bond distances range between 3.27 - 3.46Å. Also, molecule OW(1) makes another hydrogen bond with the imidazole free nitrogen N(27) of 2.77Å.

Table B1. Crystal data and structure refinement for Cometim.

Identification code	cometim
Empirical formula	C ₂₀ H ₃₃ Br ₁ Co ₁ N ₆ O _{3.5}
Formula weight	1104.73
Temperature	293(2) K
Wavelength	0.71070 Å
Crystal system	triclinic
Space group	P1 bar
Unit cell dimensions	a = 18.466(9) Å alpha = 96.27(5) deg. b = 14.936(7) Å beta = 94.12(5) deg. c = 10.111(5) Å gamma = 112.78(5) deg.
Volume	2536(2) Å ³ , Z = 2
Density (calculated)	1.447 g/cm ³
Absorption coefficient	22.86 cm ⁻¹
F(000)	1140
Crystal size	0.1 x 0.23 x 0.32 mm
Theta range for data collection	2.59 to 23.00 deg.
Index ranges	-20 ≤ h ≤ 20 -16 ≤ k ≤ 16 0 ≤ l ≤ 11
Reflections collected	7053
Independent reflections	7053 [R(int) = 0.0000]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	7053 / 0 / 808
Goodness-of-fit on F ²	1.087
Final R indices [I > 2sigma(I)]	R1 = 0.0641, wR2 = 0.1229
R indices (all data)	R1 = 0.1094, wR2 = 0.1413
Largest diff. peak and hole	0.444 and -0.499 e.Å ⁻³

Table B2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cometim. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Molecule A

	x	y	z	U eq.
Co(1)	1975(1)	3225(1)	6832(1)	34(1)
O(1)	2740(3)	4491(4)	6706(5)	42(1)
C(2)	3473(5)	4823(6)	7157(8)	45(2)
C(3)	3938(7)	5867(9)	6964(17)	77(3)
C(4)	3828(6)	4319(7)	7807(9)	51(2)
C(5)	3460(5)	3333(6)	8070(8)	45(2)
C(6)	3967(7)	2919(10)	8829(11)	64(3)
N(7)	2714(4)	2802(4)	7675(6)	38(2)
C(8)	2337(6)	1809(7)	8044(12)	63(3)
C(9)	1564(6)	1279(7)	7195(10)	54(2)
N(10)	1196(4)	1958(4)	6903(6)	37(2)
C(11)	438(5)	1667(6)	6586(8)	42(2)
C(12)	-121(8)	627(9)	6676(16)	76(3)
C(13)	110(5)	2307(7)	6163(9)	53(3)
C(14)	494(5)	3234(6)	5898(7)	45(2)
C(15)	27(8)	3792(12)	5365(19)	84(4)
N(17)	1776(3)	3729(4)	8572(6)	33(1)
C(18)	1340(5)	3233(6)	9499(8)	45(2)
C(19)	1308(4)	3889(5)	10521(8)	42(2)
C(20)	920(8)	3759(10)	11778(11)	67(3)
N(21)	1706(4)	4781(5)	10171(7)	45(2)
C(22)	1995(5)	4667(6)	9001(7)	40(2)
N(23)	2139(4)	2750(4)	5061(6)	36(2)
C(24)	2851(5)	2880(6)	4565(9)	45(2)
C(25)	2718(5)	2424(6)	3319(8)	45(2)
C(26)	3238(7)	2337(10)	2301(11)	67(3)
N(27)	1914(5)	2038(6)	2997(8)	51(2)
C(28)	1589(6)	2234(7)	4078(9)	49(2)

Molecule B

Co(1)	6921(1)	2721(1)	7400(1)	31(1)
O(1)	7947(3)	3288(3)	8412(5)	39(1)
C(2)	8446(4)	2876(6)	8382(7)	42(2)
C(3)	9254(6)	3497(9)	9151(14)	64(3)
C(4)	8295(5)	1951(6)	7793(8)	46(2)
C(5)	7567(5)	1251(5)	7114(7)	39(2)
C(6)	7496(8)	232(7)	6722(13)	59(3)
N(7)	6956(3)	1486(4)	6860(5)	32(1)
C(8)	6165(5)	752(6)	6320(9)	46(2)
C(9)	5719(6)	1234(7)	5621(9)	49(2)
N(10)	5910(3)	2214(4)	6353(6)	37(2)
C(11)	5453(4)	2687(6)	6150(8)	42(2)
C(12)	4711(7)	2213(9)	5190(14)	63(3)
C(13)	5666(6)	3651(6)	6812(8)	44(2)
C(14)	6310(5)	4197(5)	7702(8)	39(2)
C(15)	6412(9)	5194(9)	8363(17)	73(4)
O(16)	6886(3)	3947(3)	8025(5)	39(1)
N(17)	7410(3)	3235(4)	5849(5)	31(1)
C(18)	7630(5)	2782(6)	4779(8)	46(2)
C(19)	7978(5)	3421(6)	3953(8)	44(2)
C(20)	8335(8)	3307(9)	2680(11)	66(3)
N(21)	7995(4)	4300(5)	4539(7)	47(2)
C(22)	7636(5)	4152(6)	5652(8)	42(2)
N(23)	6452(3)	2204(4)	8958(6)	38(2)
C(24)	5722(5)	2120(6)	9343(8)	46(2)
C(25)	5585(5)	1634(6)	10405(8)	51(2)
C(26)	4868(10)	1300(15)	11151(17)	95(5)
N(27)	6230(5)	1429(6)	10662(8)	54(2)
C(28)	6739(5)	1767(6)	9783(8)	45(2)
Br(1)	6370(1)	9887(1)	2742(1)	66(1)
Br(2)	9291(1)	1144(1)	1028(2)	103(1)
OW1	10989(4)	1009(4)	606(6)	76(2)
OW2	7308(4)	9882(5)	-19(7)	91(2)
OW3	8355(5)	10946(6)	3887(8)	116(3)

Table B3. Bond lengths [Å] and angles [deg] for Cometim.

Molecule A

Co(1)-N(10)	1.896(6)
Co(1)-O(1)	1.897(5)
Co(1)-N(7)	1.899(6)
Co(1)-O(16)	1.908(5)
Co(1)-N(23)	1.942(6)
Co(1)-N(17)	1.952(6)
O(1)-C(2)	1.275(9)
C(2)-C(4)	1.363(11)
C(2)-C(3)	1.503(13)
C(4)-C(5)	1.428(12)
C(5)-N(7)	1.301(9)
C(5)-C(6)	1.516(12)
N(7)-C(8)	1.478(10)
C(8)-C(9)	1.483(13)
C(9)-N(10)	1.466(10)
N(10)-C(11)	1.297(9)
C(11)-C(13)	1.401(11)
C(11)-C(12)	1.512(13)
C(13)-C(14)	1.357(11)
C(14)-O(16)	1.292(9)
C(14)-C(15)	1.522(13)
N(17)-C(22)	1.311(9)
N(17)-C(18)	1.369(9)
C(18)-C(19)	1.365(10)
C(19)-N(21)	1.351(10)
C(19)-C(20)	1.498(12)
N(21)-C(22)	1.352(10)
N(23)-C(28)	1.303(10)
N(23)-C(24)	1.391(9)
C(24)-C(25)	1.323(11)
C(25)-N(27)	1.366(10)
C(25)-C(26)	1.486(11)
N(27)-C(28)	1.342(10)

Molecule B

Co(1)-N(7)	1.891(6)
Co(1)-O(16)	1.898(5)
Co(1)-N(10)	1.905(6)
Co(1)-O(1)	1.908(5)
Co(1)-N(23)	1.943(6)
Co(1)-N(17)	1.947(6)
O(1)-C(2)	1.292(8)
C(2)-C(4)	1.356(11)
C(2)-C(3)	1.515(12)
C(4)-C(5)	1.412(11)
C(5)-N(7)	1.322(9)
C(5)-C(6)	1.482(11)
N(7)-C(8)	1.465(10)
C(8)-C(9)	1.477(12)
C(9)-N(10)	1.462(10)
N(10)-C(11)	1.312(9)
C(11)-C(13)	1.411(11)
C(11)-C(12)	1.493(13)
C(13)-C(14)	1.350(11)
C(14)-O(16)	1.289(8)
C(14)-C(15)	1.499(13)
N(17)-C(22)	1.311(9)
N(17)-C(18)	1.382(9)
C(18)-C(19)	1.340(10)
C(19)-N(21)	1.368(10)
C(19)-C(20)	1.509(11)
N(21)-C(22)	1.343(10)
N(23)-C(28)	1.313(9)
N(23)-C(24)	1.393(9)
C(24)-C(25)	1.345(11)
C(25)-N(27)	1.356(11)
C(25)-C(26)	1.51(2)
N(27)-C(28)	1.333(10)

Molecule A

N(10)-Co(1)-O(1)	178.2(2)
N(10)-Co(1)-N(7)	86.8(3)
O(1)-Co(1)-N(7)	94.5(3)
N(10)-Co(1)-O(16)	95.1(2)
O(1)-Co(1)-O(16)	83.6(2)
N(7)-Co(1)-O(16)	177.6(2)
N(10)-Co(1)-N(23)	89.2(3)
O(1)-Co(1)-N(23)	89.6(2)
N(7)-Co(1)-N(23)	91.8(2)
O(16)-Co(1)-N(23)	89.8(2)
N(10)-Co(1)-N(17)	91.2(2)
O(1)-Co(1)-N(17)	90.0(2)
N(7)-Co(1)-N(17)	91.0(2)
O(16)-Co(1)-N(17)	87.5(2)
N(23)-Co(1)-N(17)	177.2(2)
C(2)-O(1)-Co(1)	125.6(5)
O(1)-C(2)-C(4)	125.1(8)
O(1)-C(2)-C(3)	114.3(8)
C(4)-C(2)-C(3)	120.6(9)
C(2)-C(4)-C(5)	126.6(8)
N(7)-C(5)-C(4)	121.5(8)
N(7)-C(5)-C(6)	120.7(9)
C(4)-C(5)-C(6)	117.8(9)
C(5)-N(7)-C(8)	120.2(7)
C(5)-N(7)-Co(1)	126.5(5)
C(8)-N(7)-Co(1)	112.8(5)
N(7)-C(8)-C(9)	108.7(8)
N(10)-C(9)-C(8)	110.8(7)
C(11)-N(10)-C(9)	122.3(7)
C(11)-N(10)-Co(1)	126.3(5)
C(9)-N(10)-Co(1)	110.9(5)
N(10)-C(11)-C(13)	121.1(7)
N(10)-C(11)-C(12)	121.0(10)
C(13)-C(11)-C(12)	117.9(9)
C(14)-C(13)-C(11)	128.2(8)
O(16)-C(14)-C(13)	124.9(8)
O(16)-C(14)-C(15)	114.9(8)
C(13)-C(14)-C(15)	120.2(9)
C(14)-O(16)-Co(1)	123.4(5)
C(22)-N(17)-C(18)	106.6(6)
C(22)-N(17)-Co(1)	123.4(5)
C(18)-N(17)-Co(1)	129.7(5)
C(19)-C(18)-N(17)	109.6(7)
N(21)-C(19)-C(18)	105.0(7)
N(21)-C(19)-C(20)	122.5(8)
C(18)-C(19)-C(20)	132.4(8)
C(19)-N(21)-C(22)	109.2(7)
N(17)-C(22)-N(21)	109.5(7)
C(28)-N(23)-C(24)	105.4(7)
C(28)-N(23)-Co(1)	126.1(5)

Molecule A (cont.)

C(24)-N(23)-Co(1)	128.4(6)
C(25)-C(24)-N(23)	110.4(8)
C(24)-C(25)-N(27)	105.3(7)
C(24)-C(25)-C(26)	133.9(9)
N(27)-C(25)-C(26)	120.6(8)
C(28)-N(27)-C(25)	108.6(8)
N(23)-C(28)-N(27)	110.2(8)

Molecule B

N(7)-Co(1)-O(16)	177.3(2)
N(7)-Co(1)-N(10)	86.6(3)
O(16)-Co(1)-N(10)	94.5(2)
N(7)-Co(1)-O(1)	95.5(2)
O(16)-Co(1)-O(1)	83.5(2)
N(10)-Co(1)-O(1)	177.2(2)
N(7)-Co(1)-N(23)	87.9(2)
O(16)-Co(1)-N(23)	89.7(2)
N(10)-Co(1)-N(23)	91.4(2)
O(1)-Co(1)-N(23)	90.6(2)
N(7)-Co(1)-N(17)	91.7(2)
O(16)-Co(1)-N(17)	90.8(2)
N(10)-Co(1)-N(17)	89.6(2)
O(1)-Co(1)-N(17)	88.4(2)
N(23)-Co(1)-N(17)	178.9(2)
C(2)-O(1)-Co(1)	123.2(5)
O(1)-C(2)-C(4)	126.1(7)
O(1)-C(2)-C(3)	114.5(8)
C(4)-C(2)-C(3)	119.3(8)
C(2)-C(4)-C(5)	127.1(7)
N(7)-C(5)-C(4)	121.3(7)
N(7)-C(5)-C(6)	120.5(8)
C(4)-C(5)-C(6)	118.2(8)
C(5)-N(7)-C(8)	122.6(6)
C(5)-N(7)-Co(1)	125.9(5)
C(8)-N(7)-Co(1)	110.7(5)
N(7)-C(8)-C(9)	109.1(7)
N(10)-C(9)-C(8)	109.6(7)
C(11)-N(10)-C(9)	121.1(7)
C(11)-N(10)-Co(1)	126.7(5)
C(9)-N(10)-Co(1)	111.7(5)
N(10)-C(11)-C(13)	120.5(7)
N(10)-C(11)-C(12)	120.0(8)
C(13)-C(11)-C(12)	119.5(8)
C(14)-C(13)-C(11)	128.0(8)
O(16)-C(14)-C(13)	125.1(7)
O(16)-C(14)-C(15)	114.6(9)
C(13)-C(14)-C(15)	120.2(9)
C(14)-O(16)-Co(1)	124.8(5)
C(22)-N(17)-C(18)	104.8(6)
C(22)-N(17)-Co(1)	124.6(5)
C(18)-N(17)-Co(1)	130.6(5)
C(19)-C(18)-N(17)	111.0(7)
C(18)-C(19)-N(21)	104.9(7)
C(18)-C(19)-C(20)	132.0(8)
N(21)-C(19)-C(20)	123.1(8)
C(22)-N(21)-C(19)	108.2(7)
N(17)-C(22)-N(21)	111.1(7)
C(28)-N(23)-C(24)	106.4(6)
C(28)-N(23)-Co(1)	125.2(5)

Molecule B (cont.)

C(24)-N(23)-Co(1)	128.0(5)
C(25)-C(24)-N(23)	109.2(7)
C(24)-C(25)-N(27)	105.1(7)
C(24)-C(25)-C(26)	130.5(10)
N(27)-C(25)-C(26)	124.4(10)
C(28)-N(27)-C(25)	110.2(8)
N(23)-C(28)-N(27)	109.1(8)

Symmetry transformations used to generate equivalent atoms

Table B4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cometim.
The anisotropic displacement factor exponent takes the form
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

Molecule A

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co(1)	37(1)	32(1)	35(1)	7(1)	10(1)	15(1)
O(1)	31(3)	42(3)	54(3)	17(3)	13(3)	12(3)
C(2)	43(5)	46(5)	52(5)	14(4)	21(4)	22(4)
C(3)	48(7)	60(8)	103(11)	17(7)	6(7)	-1(6)
C(4)	37(6)	59(6)	54(6)	-2(5)	12(5)	17(5)
C(5)	46(5)	59(6)	40(5)	2(4)	6(4)	32(5)
C(6)	62(7)	103(9)	52(6)	28(6)	19(6)	52(7)
N(7)	50(4)	48(4)	31(4)	8(3)	13(3)	34(4)
C(8)	65(7)	51(6)	92(8)	29(6)	17(6)	38(6)
C(9)	65(7)	30(5)	68(7)	7(5)	21(6)	17(5)
N(10)	47(4)	37(4)	34(4)	9(3)	12(3)	23(3)
C(11)	38(5)	40(5)	39(5)	2(4)	12(4)	5(4)
C(12)	67(8)	55(7)	86(10)	16(7)	15(8)	-1(6)
C(13)	19(5)	72(7)	58(6)	17(5)	10(4)	4(5)
C(14)	46(5)	57(6)	35(5)	14(4)	15(4)	19(5)
C(15)	47(7)	99(11)	118(12)	51(11)	3(8)	33(7)
O(16)	33(3)	41(3)	47(3)	12(2)	9(2)	15(3)
N(17)	36(4)	29(4)	38(4)	1(3)	9(3)	16(3)
C(18)	59(6)	31(5)	43(5)	3(4)	11(4)	15(4)
C(19)	39(5)	31(4)	42(5)	3(4)	10(4)	-1(4)
C(20)	85(9)	60(8)	47(7)	5(6)	23(6)	17(7)
N(21)	53(5)	30(4)	45(5)	-7(4)	3(4)	14(4)
C(22)	49(5)	37(5)	29(4)	0(4)	11(4)	14(4)
N(23)	44(4)	37(4)	32(4)	8(3)	12(3)	19(3)
C(24)	41(5)	56(6)	41(5)	5(4)	11(5)	23(5)
C(25)	48(5)	54(5)	36(5)	7(4)	18(4)	20(4)
C(26)	76(8)	98(9)	51(7)	26(6)	40(6)	53(8)
N(27)	65(6)	49(5)	35(4)	-2(4)	10(4)	19(4)
C(28)	41(6)	59(6)	43(6)	5(4)	11(5)	15(5)

Molecule B

Co(1)	33(1)	28(1)	31(1)	3(1)	7(1)	13(1)
O(1)	37(3)	36(3)	44(3)	1(2)	2(2)	18(2)
C(2)	40(5)	60(6)	36(5)	20(4)	11(4)	27(4)
C(3)	37(6)	75(8)	78(8)	-8(6)	-1(5)	26(6)
C(4)	52(6)	56(6)	48(5)	4(4)	12(4)	41(5)
C(5)	56(5)	29(4)	32(4)	3(3)	8(4)	19(4)
C(6)	81(8)	42(6)	69(8)	9(6)	15(7)	39(6)
N(7)	43(4)	27(3)	29(3)	5(3)	9(3)	15(3)
C(8)	57(6)	27(5)	40(5)	-3(4)	7(5)	4(5)
C(9)	51(6)	53(6)	38(5)	-5(4)	-8(5)	21(5)
N(10)	35(4)	35(4)	30(3)	1(3)	6(3)	4(3)
C(11)	33(5)	61(6)	39(5)	27(4)	10(4)	23(4)
C(12)	46(7)	61(7)	78(9)	17(6)	-15(6)	19(6)
C(13)	51(6)	47(6)	46(5)	13(4)	10(5)	29(5)
C(14)	46(5)	36(5)	45(5)	14(4)	16(4)	24(4)
C(15)	63(9)	47(7)	115(12)	-3(7)	1(8)	35(7)
O(16)	39(3)	28(3)	46(3)	-1(2)	1(2)	13(2)
N(17)	39(4)	26(3)	30(3)	6(3)	7(3)	14(3)
C(18)	70(6)	30(5)	44(5)	1(4)	22(4)	24(5)
C(19)	51(5)	41(5)	47(5)	13(4)	13(4)	21(4)
C(20)	93(9)	82(8)	48(6)	27(6)	39(6)	52(8)
N(21)	55(5)	39(4)	49(5)	18(4)	12(4)	15(4)
C(22)	58(5)	34(5)	35(5)	4(4)	13(4)	19(4)
N(23)	42(4)	41(4)	28(3)	5(3)	7(3)	15(3)
C(24)	46(5)	55(5)	49(5)	17(4)	13(4)	31(4)
C(25)	55(6)	56(6)	46(5)	7(4)	17(4)	26(5)
C(26)	109(12)	127(13)	69(11)	50(11)	55(10)	53(10)
N(27)	75(6)	59(5)	40(5)	22(4)	17(4)	34(5)
C(28)	54(6)	62(6)	31(5)	14(4)	17(4)	32(5)
Br(1)	88(1)	72(1)	51(1)	21(1)	23(1)	39(1)
Br(2)	92(1)	65(1)	147(1)	21(1)	31(1)	24(1)
OW1 72(4)	71(4)	60(4)	-6(3)	3(3)	7(4)	
OW2 110(6)	107(6)	75(5)	18(4)	20(4)	60(5)	
OW3 132(7)	116(7)	98(6)	-7(5)	6(5)	55(6)	

Table B5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Cometim.

Molecule A

	x	y	z	U eq.
H(3A)	4473(50)	6067(54)	7430(76)	51(23)
H(3B)	3770(63)	6311(82)	7431(113)	105(46)
H(3C)	3947(85)	5819(107)	6061(153)	172(73)
H(4)	4328(54)	4645(65)	7970(90)	76(33)
H(6A)	4559(72)	3445(83)	9080(112)	125(44)
H(6B)	4048(60)	2428(74)	8259(106)	98(38)
H(6C)	3746(54)	2676(66)	9581(100)	83(32)
H(8A)	2652(40)	1407(51)	7901(67)	43(21)
H(8B)	2253(85)	2058(106)	9037(154)	192(66)
H(9A)	1222(46)	661(61)	7344(77)	58(25)
H(9B)	1696(40)	1023(50)	6378(74)	41(21)
H(12A)	-616(75)	556(86)	6084(125)	133(50)
H(12B)	-247(44)	558(54)	7499(81)	44(25)
H(12C)	89(81)	262(99)	6431(140)	131(69)
H(13)	-353(38)	2052(44)	6041(59)	16(18)
H(15A)	-523(74)	3476(82)	5333(113)	122(44)
H(15B)	221(77)	4275(106)	4870(134)	139(55)
H(15C)	217(89)	4295(113)	5963(153)	146(79)
H(18)	1166(42)	2538(57)	9469(72)	52(23)
H(20A)	605(65)	3079(87)	11844(108)	109(42)
H(20B)	731(52)	4206(68)	11853(90)	69(34)
H(20C)	1311(55)	3848(67)	12468(99)	76(35)
H(21)	1888(41)	5289(52)	10543(72)	29(24)
H(22)	2278(41)	5152(52)	8480(72)	48(22)
H(24)	3302(40)	3187(48)	5048(68)	31(21)
H(26A)	3895(71)	2885(82)	2700(110)	128(41)
H(26B)	3088(70)	2492(87)	1482(131)	127(48)
H(26C)	3428(49)	1966(58)	2390(80)	44(29)
H(27)	1664(50)	1631(63)	2362(89)	65(32)
H(28)	1088(45)	2036(53)	4108(75)	49(25)

Molecule B

H(3A)	9590(59)	3333(71)	8869(99)	75(37)
H(3B)	9262(84)	3676(107)	10127(164)	181(68)
H(3C)	9443(65)	4093(86)	8774(113)	116(47)
H(4)	8744(39)	1760(47)	7987(64)	39(19)
H(6A)	7891(54)	133(66)	7083(93)	75(34)
H(6B)	7278(61)	-131(78)	5908(113)	98(42)
H(6C)	7051(62)	-292(79)	7044(105)	103(39)
H(8A)	6198(36)	306(46)	5928(63)	15(20)
H(8B)	5841(39)	401(49)	7027(70)	41(20)
H(9A)	5169(45)	866(51)	5484(70)	44(22)
H(9B)	5876(45)	1305(55)	4667(86)	66(26)
H(12A)	4423(49)	2577(59)	5041(82)	55(27)
H(12B)	4381(33)	1709(42)	5412(53)	0(16)
H(12C)	4824(112)	2239(143)	4520(190)	238(110)
H(13)	5345(36)	3882(45)	6737(62)	19(20)
H(15A)	6035(57)	5307(67)	8125(94)	74(36)
H(15B)	6868(61)	5641(73)	8309(102)	77(37)
H(15C)	6619(72)	5290(85)	9234(117)	114(53)
H(18)	7515(33)	2163(45)	4660(57)	17(17)
H(20A)	8433(54)	2772(71)	2580(92)	79(35)
H(20B)	8952(81)	3836(95)	2676(128)	157(52)
H(20C)	7953(41)	3292(51)	2042(74)	36(23)
H(21)	8216(52)	4875(67)	4220(91)	87(32)
H(22)	7612(33)	4678(44)	6221(59)	20(16)
H(24)	5414(37)	2457(45)	8848(63)	35(18)
H(26A)	4548(98)	1821(128)	10933(176)	232(80)
H(26B)	4953(57)	1471(71)	11754(82)	35(32)
H(26C)	4912(48)	695(62)	11430(90)	62(29)
H(27)	6301(34)	1108(41)	11092(58)	0(17)
H(28)	7216(36)	1688(41)	9714(58)	21(17)